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14. ABSTRACT

This document is the final report for AFOSR Grant F49620-99-1-0070, "Lattice Hydrodynamics." Under the terms of this grant, the Center for Computational Science at Boston University provided theoretical and computational support to the Lattice-Gas Theory and Computation group at the Space Vehicles Directorate of Air Force Research Laboratory (AFOSR task 2304CP). The principal research topics were the development of quantum lattice-gas models for implementation on quantum computers, and classical lattice Boltzmann models for complex fluids. Seven publications have resulted from this effort, as well as the editorship of the Proceedings of the Workshop on Quantum Computation for Physical Modeling (QCPM 2000), which was held in Falmouth, Massachusetts in October, 2000. These proceedings, edited by Bruce M. Boghosian and Jeffrey Yepez, will appear in the journal *Computer Physics Communications*. The principal results of this work are described in this report.

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Lattice Hydrodynamics
(Final Report for AFOSR Grant Number F49620-99-1-0070)

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Abstract

This document is the final report for AFOSR Grant F49620-99-1-0070, "Lattice Hydrodynamics." Under the terms of this grant, the Center for Computational Science at Boston University provided theoretical and computational support to the Lattice-Gas Theory and Computation group at the Space Vehicles Directorate of Air Force Research Laboratory (AFOSR task 2304CP). The principal research topics were the development of quantum lattice-gas models for implementation on quantum computers, and classical lattice Boltzmann models for complex fluids. Seven publications have resulted from this effort, as well as the editorship of the Proceedings of the Workshop on Quantum Computation for Physical Modeling (QCPM 2000), which was held in Falmouth, Massachusetts in October, 2000. These proceedings, edited by Bruce M. Boghosian and Jeffrey Yepez, will appear in the journal *Computer Physics Communications*. The principal results of this work are described in this report.

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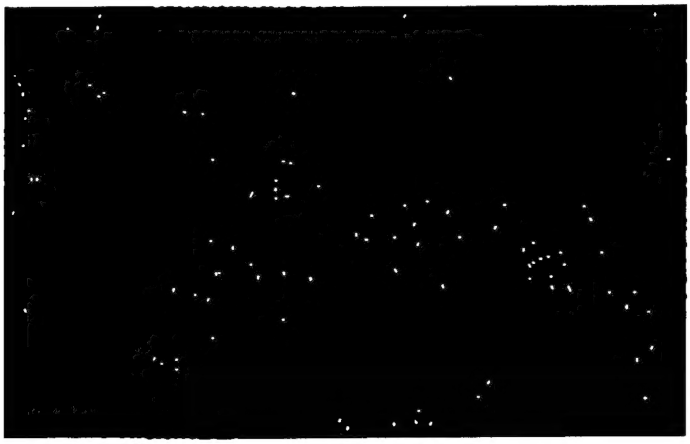

Figure 1: Two-fermion probability density

1 Principal Areas of Study

1.1 Quantum Lattice Models

Classical lattice-gas automata (LGA) are discrete dynamical systems in which a finite number of state bits are maintained at each site of a grid, and evolve synchronously according to logical rules involving the state of a given site and its neighbors. If the LGA has a total of N bits of state, it can be in any one of 2^N states. The dynamics is thus a deterministic or stochastic Markov process on these states. Since the mid 1980's, it has been known how to construct LGA whose coarse-grained behavior is that of a Navier-Stokes fluid.

Quantum lattice-gas automata (QLGA) are a generalization of LGA. Whereas an LGA with N bits can be in any one of 2^N distinct states, a QLGA can be in a complex superposition of *all* of those 2^N states – although conservation of mass (and momentum if appropriate) restricts the evolution to particular sectors of the full Hilbert space. The moduli squared of these complex amplitudes may be thought of as the probability that the system is in the corresponding state. As these amplitudes evolve according to unitary transformations, they can *interfere* with one another, giving rise to behavior that is not possible with classical lattice-gas automata.

The AFRL group led by Jeffrey Yepez is currently engaged in a program of realizing QLGA using nuclear magnetic resonance (NMR) apparatus. The NMR apparatus used is very nearly "off the shelf"; it required very little modification from those used for medical imagery. The idea is that, by placing certain organic molecules in a strong magnetic field, one can control the spin states of various nuclear spins using radio frequency. The nuclear spins are coupled by the electronic structure of the molecule. Because the NMR sample contains order 10^{18} molecules, the measured signal effectively averages over these, yielding a high signal-to-noise ratio. (It is to be emphasized, however, that only spins within the same molecule enter into a single computation.) The apparatus is able to localize subsets of the molecules according to their spatial position by using field gradients.

During the granting period covered by this report, Bruce Boghosian and Jeffrey Yepez have coauthored a paper entitled "An Efficient and Accurate Quantum Lattice-Gas Model for the Many-Body Schrödinger Wave Equation," which will appear in the journal *Computer Physics Communications* in 2001 [1]. This paper contains the principal results obtained on the QLGA project during this reporting period; we described and simulated a quantum lattice-gas model for a system of particles governed by the nonrelativistic Schrödinger equation. The paper also contains the first two-fermion simulations of Schrödinger's equation using the quantum lattice-gas algorithm. An illustration of the two-particle probability density versus position is presented in Fig. 1.

In this work, we also measured the accuracy of the method, as a function of spatial resolution [1]. We found that the method was fourth-order accurate in space. More significantly, however, we found that the emergent Schrödinger evolution is *not* exactly unitary, as had been previously reported [2], even for

the simplest case of one particle in one dimension. In that case, the dynamical variables are $\psi_+(x,t)$ and $\psi_-(x,t)$, and the quantity that satisfies the Schrödinger equation is

$$\psi(x,t) = \psi_+(x,t) + \psi_-(x,t).$$

Because the method follows unitary evolution, it is true that

$$\sum_x \sum_{j=\pm} |\psi_j|^2 = 1$$

for all t, but it does not follow from this that

$$\sum_x |\phi(x,t)|^2 = 1.$$

In fact, the latter is true only in the continuum limit. In other words, while the QLGA is unitary, the emergent Schrödinger equation is not.

These observations have shaped the direction of our future research on QLGA. We are currently adopting a new model for the QLGA that will yield *perfectly* unitary Schrödinger evolution, by casting an operator-splitting approach into the form of a QLGA.

Finally, in October of 2000, Bruce Boghosian participated in the organization of the meeting QCPM 2000 (Quantum Computing for Physical Modelling). Details about this meeting can be found on the meeting web page:

`http://xyz.plh.af.mil/QCPM2000/QCPM2000_dlab.html`

Jeffrey Yepez and Bruce Boghosian are currently coediting the proceedings for this meeting, which will appear in the journal *Computer Physics Communications*. A partial table of contents for these proceedings appears as an appendix to this report.

1.2 Entropic Lattice Boltzmann Models

Over the last ten years, lattice BGK methods (a particular kind of lattice Boltzmann model) has emerged as one of the more important and successful methodologies of computational fluid dynamics. As has been noted by several authors, however, lattice BGK methods lack an H-theorem, and are plagued by a variety of ill-understood numerical instabilities. In recent work, we have demonstrated a generalization of the BGK technique that makes it possible to reintroduce an H-theorem in many cases. During the period of this grant, we have completed and published a general program for the construction of "entropically stabilized" lattice Boltzmann models, and illustrated its application to several example problems [3].

The crux of the idea is to encourage the model builder to specify an appropriate H function (Lyapunov function) for the model, rather than try to blindly dictate an equilibrium state, as is done for BGK models. Of course, specifying a form for H determines the equilibrium distribution, but it also governs the *approach* to this equilibrium. It can therefore be used to control the stability properties of the model. It should be emphasized that the presence of a Lyapunov function guarantees the *nonlinear* stability of the model, which is a much stronger condition than linear stability.

In earlier work, under AFOSR grant number F49620-95-1-0285, we showed that collision operators that are constructed to increase H defined in this way are similar in form to the lattice BGK collision operators, except that their relaxation parameter may depend on the current state. As a result, the transport coefficients may have a certain minimum value in models of this type but these minimum values are often actually zero. The results from that study are illustrated in Fig. 2, which shows the decay of the amplitude of an initially sinusoidal density profile in a simple entropic lattice Boltzmann model of diffusion. Table 1 then shows the theoretical value of the diffusion versus the value measured from numerical experiments. We see that the agreement is good for values of the diffusivity (in lattice units) greater than one part in 10^4.

In the present work, we have demonstrated that this makes possible the construction of fully explicit, perfectly conservative, absolutely stable algorithms with arbitrarily small transport coefficients. In fact, we have showed that the ultimate limitation to the application of these algorithms for very small transport coefficients come from considerations of accuracy, rather than stability. We have created entropically stabilized

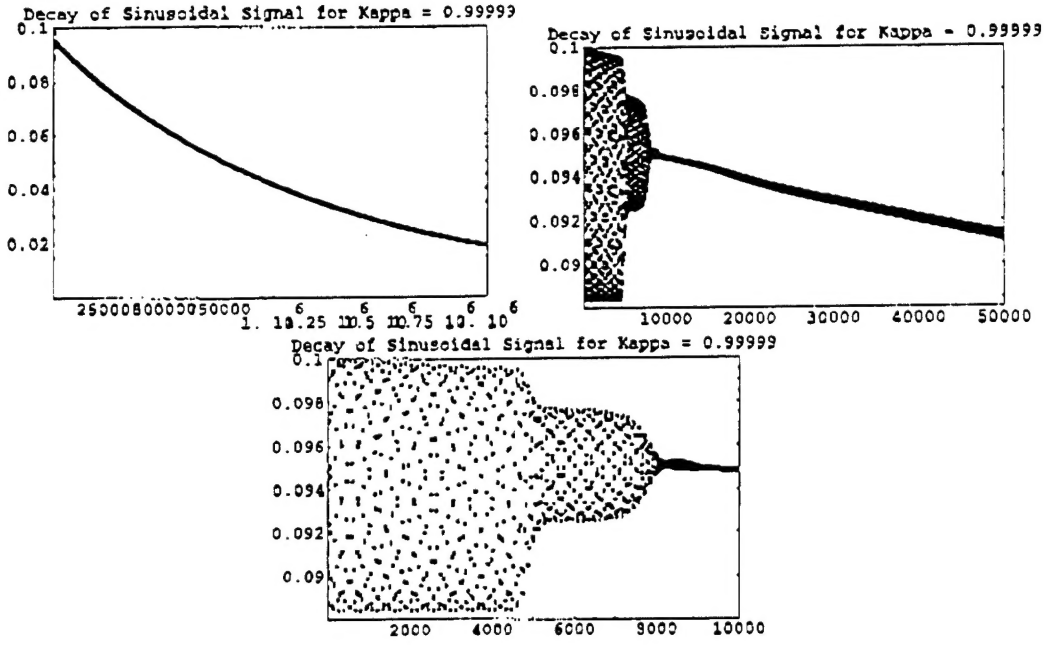

Figure 2: **Decay of sinusoidal density profile** for $\kappa = 0.99999$

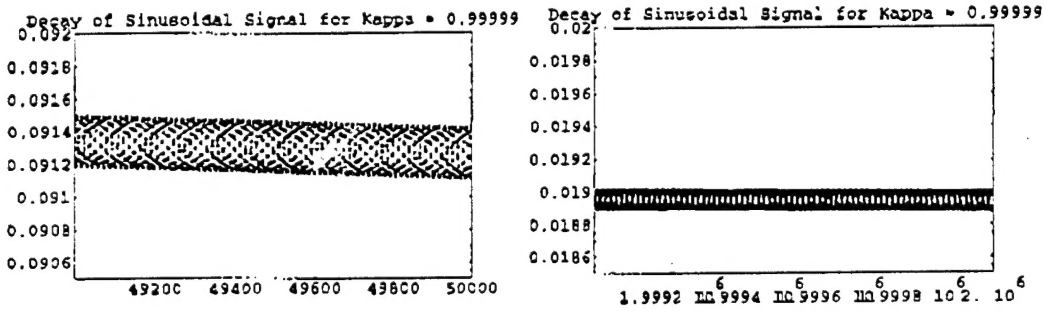

Figure 3: **Decay of sinusoidal density profile** for $\kappa = 0.99999$

κ	D_{theory}	D_{meas}
0.9	1.852×10^{-2}	1.75364×10^{-2}
0.99	1.684×10^{-3}	1.67419×10^{-3}
0.999	1.668×10^{-4}	1.66674×10^{-4}
0.9999	1.667×10^{-5}	1.66198×10^{-5}
0.99999	1.667×10^{-6}	2.28751×10^{-6}

Table 1: **Theoretical and measured values of the diffusivity** for various values of κ.

lattice Boltzmann models of two dimensional Navier-Stokes flow that are stable for values of the viscosity in lattice units that are more than two orders of magnitude smaller than what is possible in lattice BGK simulations. Since computational complexity scales as Reynolds number cubed, this implies a six-order of magnitude decrease in the number of site updates necessary. The entropically stabilized algorithm requires more than two orders of magnitude more floating-point operations per site update. Nevertheless, the net result would be a three-order of magnitude improvement in computational complexity for a given calculation – *if stability were the only limiting factor.* In practice, other accuracy considerations may enter; on the other hand, the entropically stabilized algorithm may well be valid beyond the point where the smallest eddies are on the order of the grid size. In some sense, entropic stabilization may constitute a new kind of subgrid turbulence model, and this is driving the direction of present research on this topic. Our publication gives more details on this issue [3].

In order to conduct these studies, we had to develop algorithms for efficient site updates using the entropically stabilized algorithm. There are two principal algorithmic problems that enter for models of fluids in two and three dimensions. First, it is first necessary to find the equilibrium distribution for given values of the conserved quantities. Second, it is necessary to find the minimum value of the collision parameter $\tau_{\min}$ for which the step will be stable. The value of the collision parameter τ actually used is then $\tau_{\min}/\kappa$, where $\kappa < 1$. We have shown that the transport coefficient goes to zero as $\kappa \to 1$.

To solve the first of these problems, we noted that the equilibrium distribution could be perturbatively expanded in Mach number [3]. Subsequent to the publication of our paper, we found that if this Mach-number-expanded equilibrium is used as the initial guess in a Newton-Raphson solution for the exact equilibrium, the solution will converge in *one pass* of the Newton-Raphson algorithm for Mach numbers less than 0.3.

At the time of publication of the paper [3], we had no similar Mach number expansion of $\tau_{\min}$. In subsequent work, we found that the difficulty stemmed from the nonanalyticity of $\tau_{\min}$ at the equilibrium point. This is illustrated for the diffusion model in Fig. 4. We were then able to construct rational approximations – Padé approximations – to $\tau_{\min}$ that could likewise be used as the initial guess in a Newton-Raphson iteration for the exact solution. As with the equilibrium point, we have found that such Newton-Raphson solutions converge in one step, thereby making possible efficient entropic lattice-Boltzmann simulations. These latter algorithmic advances will be reported on in a future publication [4].

2 Conclusions

We have described the program of activity of the lattice-gas research collaboration between the Boston University Center for Computational Science and the Space Vehicles Directorate of AFRL (under AFOSR task 2304CP). This collaboration has centered on three major areas of study: (i) lattice-fluid models for droplet formation, (ii) entropic lattice Boltzmann models, and (iii) quantum lattice-gas automata. We have provided a detailed account of the principal new results in all three of these areas. Nine publications have resulted from this effort, as well as the sponsorship of the Seventh International Conference on Discrete Models for Fluid Mechanics, and the preparation of the proceedings of that meeting as a special issue of the *International Journal of Modern Physics C.*

References

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[2] B.M. Boghosian, W. Taylor, *Int. J. Mod. Phys. C* 8 (1997) 705.

[3] B.M. Boghosian, J. Yepez, A. Wagner, P.V. Coveney, "Entropic Lattice Boltzmann Models,"

[4] B.M. Boghosian, J. Yepez, in preparation (2001).

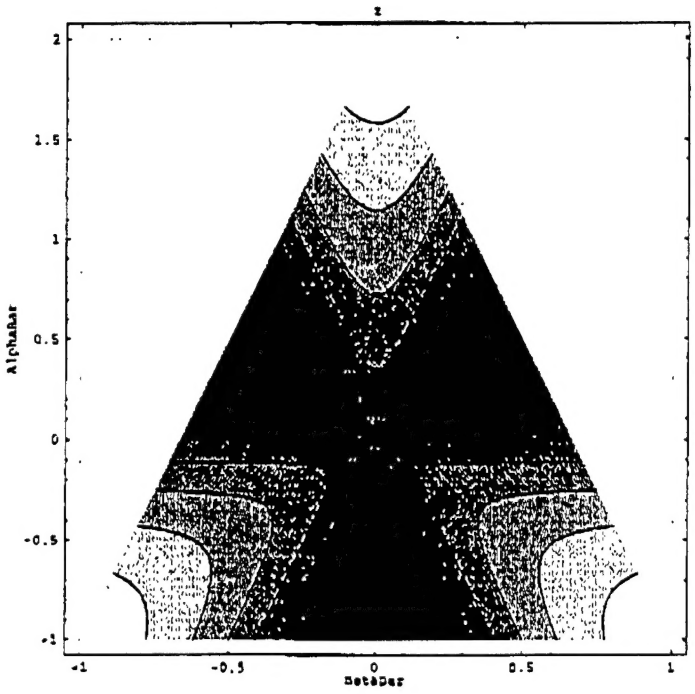

Figure 4: Minimum tau as function in allowed polytope of states. Note nonanalyticity at equilibrium point.

A Publications

The following seven publications coauthored by Bruce M. Boghosian were related to the topic of this grant proposal, and were published during the time period of the grant:

1. B.M. Boghosian, J. Yepez, P.V. Coveney, A.J. Wagner, "Entropic Lattice Boltzmann Methods," *Proc. Roy. Soc. Lon. A* **457** (2001) 717-766. cond-mat/0005260

2. M. Nekovee, P.V. Coveney, H. Chen, B.M. Boghosian, "A Lattice-Boltzmann Model for Interacting Amphiphilic Fluids," *Phys. Rev. E* **62** (2000) 8282-8294. cond-mat/0006319

3. Francis J. Alexander, Bruce M. Boghosian, Richard C. Brower, S. Roy Kimura, "Fourier Acceleration of Langevin Molecular Dynamics," to appear *Phys. Rev. E* (2001). cond-mat/0001418

4. B.M. Boghosian, C. Chow, T. Hwa, "Hydrodynamics of the Kuramoto-Sivashinsky Equation in Two Dimensions," *Phys. Rev. Lett.* **83** (1999) 5262-5265. cond-mat/9911069

5. B.M. Boghosian, P.V. Coveney, "A Particulate Basis for an Immiscible Lattice-Gas Model," *Comp. Phys. Comm.* **129** (2000) 46-55. cond-mat/9911340

6. H. Chen, B.M. Boghosian, P.V. Coveney, M. Nekovee, "A Lattice Boltzmann Model of Ternary Amphiphilic Fluids," *Proc. Roy. Soc. London A* **456** (2000) 2043-2057. cond-mat/9910369

7. B.M. Boghosian, P.V. Coveney, P.J. Love, "A Three-Dimensional Lattice-Gas Model for Amphiphilic Fluid Dynamics," *Proc. Roy. Soc. Lon. A* **456** (2000) 1431-1454. cond-mat/9907298

B Invited Talks and Presentations

The following invited talks and presentations by Bruce M. Boghosian were related to the topic of this grant proposal, and were presented during the time period of the grant:

1. Speaker, "Symposium Celebrating the Tenth Anniversary of the Center for Computational Science," Boston University (17 November, 2000).
2. Speaker, Greater Boston Statistical Mechanics Meeting, Brandeis University (14 October 2000).
3. Member of Scientific Program Committee, "Ninth International Conference on Discrete Models for Fluid Dynamics" Santa Fe, New Mexico (21-25 August, 2000).
4. Speaker, Gordon Conference on Computational Physics Education, Plymouth, New Hampshire (11-16 June, 2000).
5. Speaker, Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio (30 May, 2000).
6. Minisymposium speaker, "Role of Curvature and Hydrodynamics in Soft and Biological Matter," Third SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, Pennsylvania (22-24 May, 2000).
7. Colloquium speaker, Department of Physics, Clark University, Worcester, Massachusetts (27 April, 2000).
8. Colloquium speaker, Department of Physics, Boston University, Boston, Massachusetts (4 April, 2000).
9. Speaker, "Recent Developments in Computer Simulation Studies in Condensed Matter Physics," Center for Simulational Physics, Department of Physics and Astronomy, University of Georgia, Athens, Georgia (21-25 February, 2000).
10. Colloquium speaker, Department of Mathematics, Tufts University, Medford, Massachusetts (17 February, 2000).
11. Colloquium speaker, Department of Mathematics, Worcester Polytechnic Institute, Worcester, Massachusetts (3 February, 2000).
12. Seminar speaker, Department of Applied Mathematics, University of North Carolina, Chapel Hill, North Carolina (5 November, 1999).
13. Seminar speaker, Department of Chemistry, University of London, Queen Mary and Westfield College, London, United Kingdom (9 July, 1999).
14. Seminar speaker, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico, 10 June 1999.
15. Organizing Committee member, NIST CTCMS Workshop on Hybrid Methods in Multiscale Modeling of Materials, 12-14 May 1999.
16. Speaker, Molecular Simulation '99, Advances in Mesoscale Simulation Methodology, Web-based real-time conference at URL `http://molsim.vei.co.uk/` (27 April 1999).
17. Seminar speaker, Department of Mechanical Engineering, Massachusetts Institute of Technology (6 April 1999).

C Honors and Awards

Bruce Boghosian was elected a Fellow of the American Physical Society in 2000. He was also invited to join the editorial advisory board of the journal *Physica A*. He remains on the editorial boards of the *International Journal of Modern Physics C*, and of *Computers in Science and Engineering*.

D Proceedings of the Workshop on Quantum Computation for Physical Modeling (QCPM 2000)

This is a list of the publications that will appear in the Proceedings of the Workshop on Quantum Computation for Physical Modeling (QCPM 2000), held in Falmouth, Massachusetts in October, 2000. These proceedings, edited by Bruce M. Boghosian and Jeffrey Yepez, will appear in the journal *Computer Physics Communications*.

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